Comparison of ENDF71x and ENDF70 Using ICSBEP Criticality Benchmarks in MCNP6

Steven J. Gardiner, Jeremy Lloyd Conlin, A. C. Kahler, D. Kent Parsons

Los Alamos National Laboratory, Los Alamos, NM, 87544
sgardiner@lanl.gov, jlconlin@lanl.gov

INTRODUCTION

The Nuclear Data Team at Los Alamos National Laboratory (LANL) has recently prepared [1, 2] an ACE-format, continuous-energy neutron data library called ENDF71x. This library is based on ENDF/B-VII.1 [3] and includes data for 423 nuclides at 7 temperatures: 0.1, 250, 293.6, 600, 900, 1200, and 2500 K. ENDF71x expands upon its ENDF/B-VII.0-based predecessor, ENDF70 [4], by adding 32 new evaluations and 2 new temperatures. The ENDF71x library is scheduled for release, through RSICC, with the first production version of MCNP6 [5].

Members of the LANL Nuclear Data Team have conducted extensive tests in an effort to verify ENDF71x for use with MCNP [6]. To validate ENDF71x against experimental measurements, we have performed calculations of criticality benchmarks using a suite of 717 MCNP models. These models, created by A. "Skip" Kahler [7] and Russ Mosteller [8], are based on experiments selected from the International Criticality Safety Benchmark Evaluation Project's International Handbook of Evaluated Criticality Benchmark Experiments (ICSBEP Handbook) [9]. Our suite of 717 benchmarks is identical to that used in an earlier study by Relson, et al. [10].

Kahler, et al. [7] and van der Marck [11] have already performed similar sets of criticality calculations to test preliminary collections of ENDF/B-VII.1-based ACE files. However, because ENDF71x will serve as the officially supported ENDF/B-VII.1-based ACE library for use with MCNP, direct validation of ENDF71x is warranted.

To begin our criticality calculations, we ran all of the simulations in this validation suite using ENDF71x data in MCNP6-1.0. We then repeated these calculations using ENDF70. With the exception of some minor changes that were needed to make the switch between the two data libraries, the input files used in each set of MCNP simulations were identical. The 2 runs of our 717-benchmark validation suite required approximately 6851 CPU hours to complete.

In this summary, we will briefly discuss and compare the calculated eigenvalues that were obtained from these 2 sets of criticality calculations. A more detailed treatment of these results will be published in the near future.

VALIDATION SUITE

The ICSBEP Handbook identifies its benchmark models using codes of the form FUEL-CHEM-SPEC-EVAL.CASE, where:

FUEL identifies the primary fuel in the system (PU for ^{239}Pu, U233 for ^{233}U, MIX for a combination of ^{235}U and ^{239}Pu, and HEU, IEU, and LEU for highly-, intermediate-, and low-enriched uranium);

CHEM represents the chemical composition of the fuel (MET for metal, COMP for compound, SOL for solution, and MISC for other compositions);

SPEC describes the flux spectrum (FAST when 50% of the neutron flux is above 100 keV, THERM when 50% of the flux is below 0.625 eV, INTER when 50% of the flux is between those limits, and MIXED for all other spectra);

EVAL is a number that identifies the experiment; and

CASE is a number that identifies the configuration.

In this summary, we will refer to all of the benchmarks that share the same fuel, composition, and flux spectrum codes as a benchmark group. We will also occasionally abbreviate the benchmark names using the first letter or nonzero digit of each identifier, e.g., HEU-SOL-THERM-001.1 becomes HST1.1.

Table I shows the number of models from each benchmark group that are included in our validation suite. In each criticality calculation, we used between 500 and 5000 active cycles with 10,000 neutron histories per cycle.

Benchmark Group	Number of Benchmarks
HEU-COMP-INTER	1
HEU-MET-FAST	174
HEU-MET-INTER	4
HEU-MET-MIXED	5
HEU-SOL-THERM	46
IEU-COMP-THERM	1
IEU-MET-FAST	16
LEU-COMP-THERM	101
LEU-SOL-THERM	22
MIX-COMP-THERM	6
MIX-MET-FAST	34
PU-COMP-INTER	1
PU-MET-FAST	43
PU-SOL-THERM	122
U233-COMP-THERM	2
U233-MET-FAST	10
U233-SOL-INTER	26
U233-SOL-THERM	103

TABLE I. Benchmarks in our Criticality Validation Suite

RESULTS

For the problems included in our benchmark suite, the calculated eigenvalues that we obtained using ENDF71x and ENDF70 generally agreed. Figure 1 shows the difference in C/E value (the ratio of the MCNP calculated eigenvalue to the experimental model eigenvalue) between the ENDF71x and ENDF70

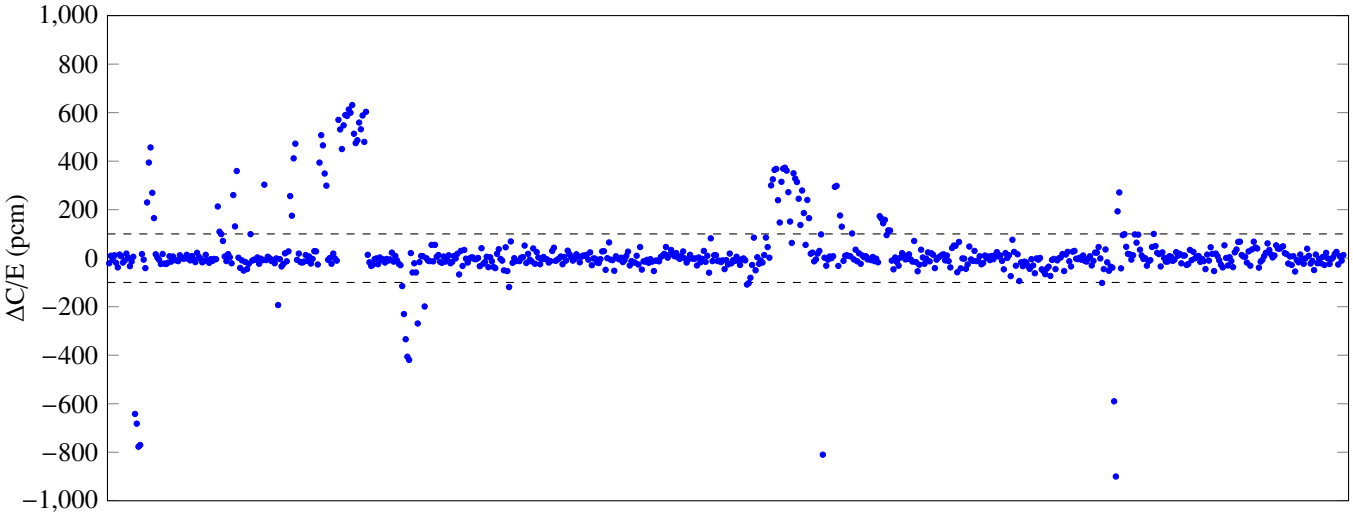

Fig. 1. Differences in C/E values ($C/E_{ENDF71x} - C/E_{ENDF70}$)

calculations for each benchmark. Data points that fall between the two dashed lines represent benchmarks whose ENDF71x and ENDF70 C/E values differed by less than 100 pcm. The overwhelming majority (about 87%) of the benchmarks in our suite gave pairs of C/E values that agreed this closely. Nearly all of the larger differences can be attributed to changes made to the data for 3 elements between ENDF/B-VII.0 and ENDF/B-VII.1: beryllium (70% of the larger differences), titanium (10%), and tungsten (8%).

Figure 2 summarizes the results of our calculations. The C/E values obtained using ENDF71x and ENDF70 are plotted as blue and red points, respectively, while experimental uncertainties for each benchmark are shown as gray bars. While the results from ENDF71x and ENDF70 generally agree with the benchmark model predictions, many notable discrepancies (including a long-standing overprediction of Pu solution eigenvalues [7]) remain.

To obtain a quantitative measure of the level of disagreement between the benchmark model eigenvalues and the calculated eigenvalues that we obtained using ENDF71x and ENDF70, we performed a large number of simultaneous hypothesis tests. In each hypothesis test, we assumed that each of eigenvalues being compared came from a normal distribution. For a few of the benchmarks that we used, the ICSBEP Handbook either did not give an experimental uncertainty (HMF4) or gave an asymmetric uncertainty (HMF57 and HMF58). When an experimental uncertainty was not given for a benchmark, we omitted the benchmark from our series of hypothesis tests comparing ENDF71x calculated eigenvalues with experiment. When an asymmetric uncertainty was given, we used a symmetric uncertainty equal to the larger of the plus and minus uncertainties.

Table II lists counts from each benchmark group of the number of calculated ENDF71x eigenvalues that differed from the experimental eigenvalue and from the calculated ENDF70 eigenvalue at the Bonferroni-adjusted 5% significance level [12]. Out of the 101 benchmarks for which the ENDF71x and ENDF70 eigenvalues differed at this significance level, the ENDF71x eigenvalues were larger than the ENDF70 eigenvalues for all 80 benchmarks that contained beryllium, while they were smaller than the ENDF70 eigenvalues for the 21 other benchmarks.

Benchmark Group	# Different from Benchmark Model	# Different from ENDF70 Calculation
HEU-MET-FAST	10	49
HEU-MET-INTER	2	0
HEU-MET-MIXED	0	2
HEU-SOL-THERM	0	1
IEU-MET-FAST	1	0
LEU-COMP-THERM	4	1
LEU-SOL-THERM	2	0
MIX-MET-FAST	1	24
PU-MET-FAST	0	11
PU-SOL-THERM	10	3
U233-MET-FAST	1	5
U233-SOL-INTER	5	5
U233-SOL-THERM	5	5

TABLE II. Counts of benchmarks from each group whose ENDF71x calculated k_{eff} differed from the benchmark model k_{eff} and the ENDF70 calculated k_{eff} at the 5% percent significance level

For our criticality benchmark suite as a whole, both ENDF71x and ENDF70 tended to overestimate the experimental eigenvalues. The mean C/E values, root mean square deviations from unity (RMSD = $\sqrt{\frac{\sum_{i=1}^{n}(C/E_i-1)^2}{n}}$, where $n = 717$ is the number of benchmarks in our suite), and mean absolute deviations from unity (MAD = $\frac{1}{n}\sum_{i=1}^{n}|C/E_i - 1|$) obtained using ENDF71x and ENDF70 for the population of criticality benchmarks in our suite are compared in Table III. The higher average C/E value that we obtained using ENDF71x is largely

due to a significant upward shift of nearly all of the calculated eigenvalues for benchmarks containing beryllium. Although this shift noticeably improves the accuracy of the calculated eigenvalues for some beryllium-containing benchmarks (e.g., HMF66, HMF77), others (MMF7 in particular) yield considerably poorer results.

The smaller RMSD and MAD values for ENDF71x show that, on average, ENDF71x gives C/E values that are slightly closer to unity than those given by ENDF70 for the benchmarks in our suite. However, these two metrics depend on our choice of benchmarks. Therefore, they should only be interpreted as rough measures of the general performance of these nuclear data libraries.

Library	Mean C/E	RMSD	MAD
ENDF71x	1.00061	0.00626	0.00420
ENDF70	1.00039	0.00638	0.00430

TABLE III. Mean C/E values, Root Mean Square Deviations (RMSD) from unity, and Mean Absolute Deviations (MAD) from unity for our benchmark suite calculations

CONCLUSION

For our suite of 717 MCNP criticality benchmarks, the ENDF71x and ENDF70 libraries generally produce comparable calculated eigenvalues. In cases where the ENDF71x and ENDF70 eigenvalues significantly differ, the disagreement between the two libraries can usually be attributed to changes in the ENDF/B evaluations for 3 elements: beryllium, titanium, and tungsten.

Both libraries give results for our benchmarks that usually agree well with the experimental predictions. Although ENDF71x sometimes gives results that are less accurate than ENDF70, the ENDF71x C/E values are, on average, slightly closer to unity than the ENDF70 C/E values.

ACKNOWLEDGMENTS

We thank Russ Mosteller, Forrest Brown, and Brian Kiedrowski for contributing MCNP input files from their Expanded Validation Suite [8] for this study. We also thank J. Tim Goorley and Forrest Brown for their direct support of this work.

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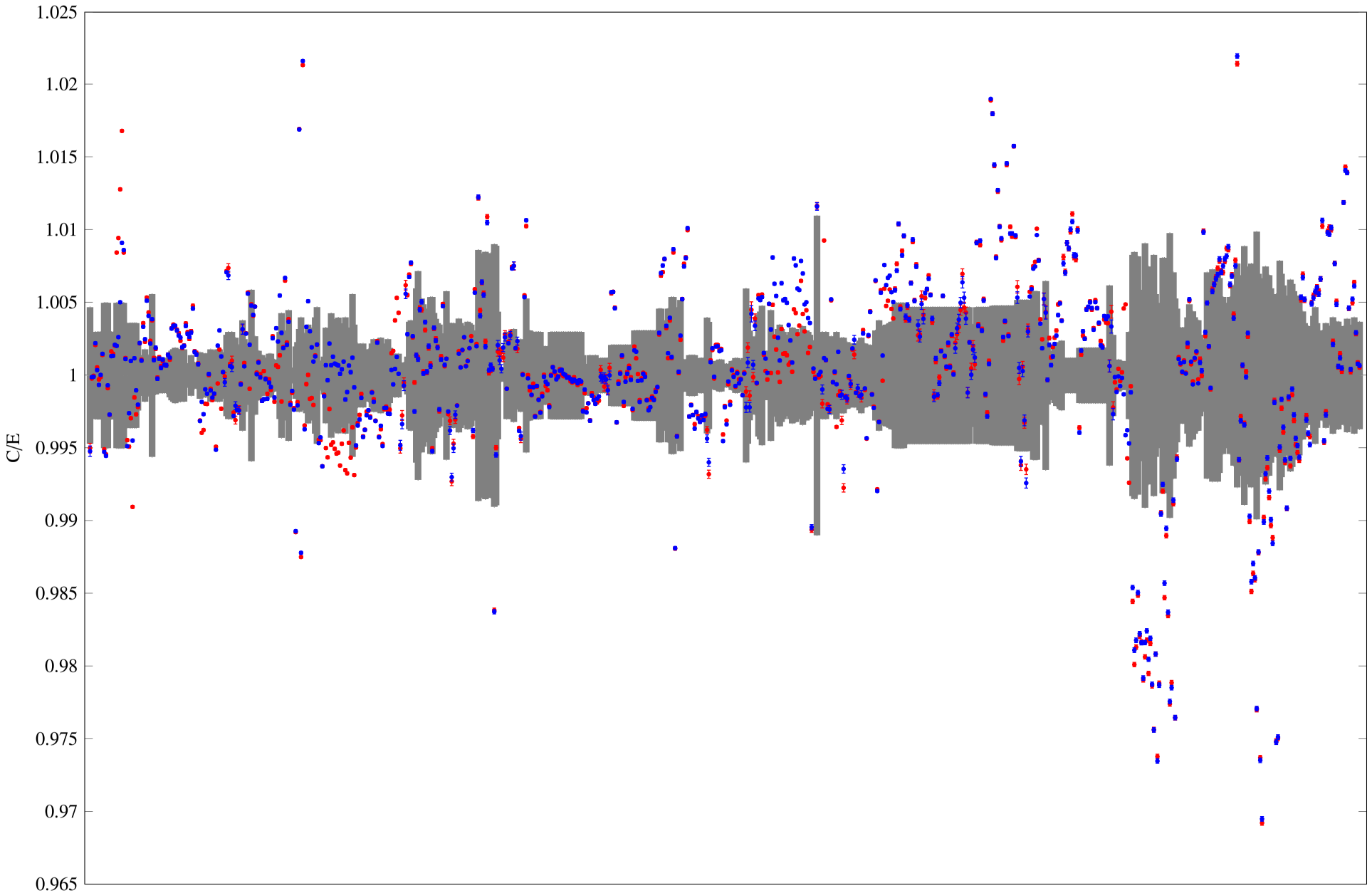

Fig. 2. Benchmark model uncertainties (gray) and C/E values for ENDF71x (blue) and ENDF70 (red) for all 717 problems in our benchmark suite